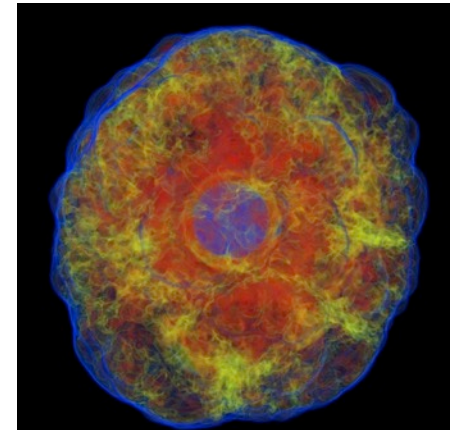
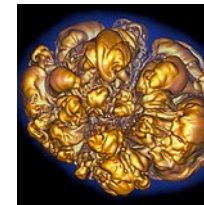
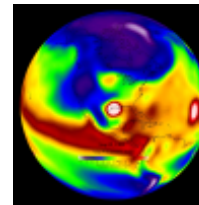
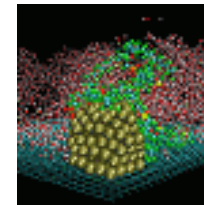
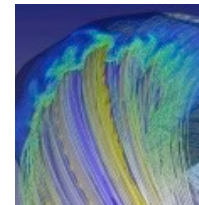
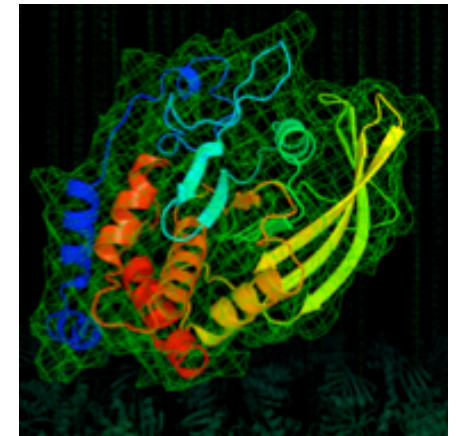
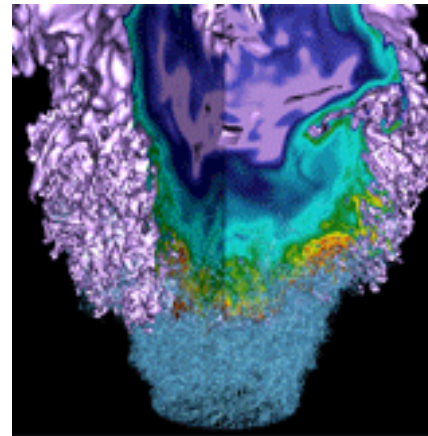


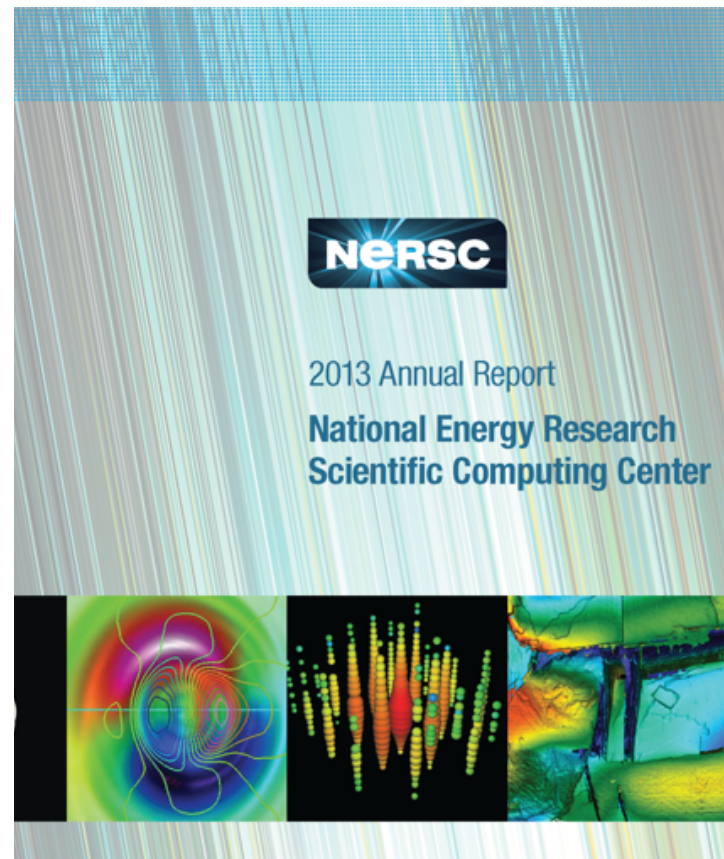
NERSC Overview



Rebecca Hartman-Baker
NERSC User Engagement Group

NUG 2016 New User Training
March 22, 2016

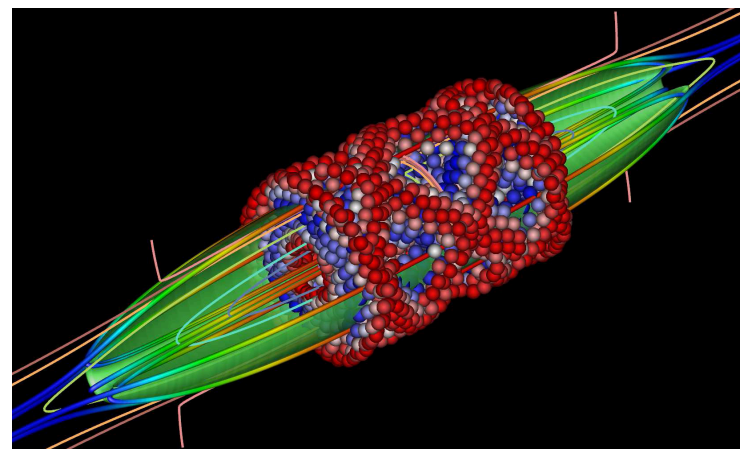
- **National Energy Research Scientific Computing Center**
 - Established 1974, first unclassified supercomputer center
 - Original mission: to enable computational science as a complement to magnetically controlled plasma experiment
- Today's mission: ***Accelerate scientific discovery at the DOE Office of Science through high performance computing and extreme data analysis***
- A national user facility



Today's Talk

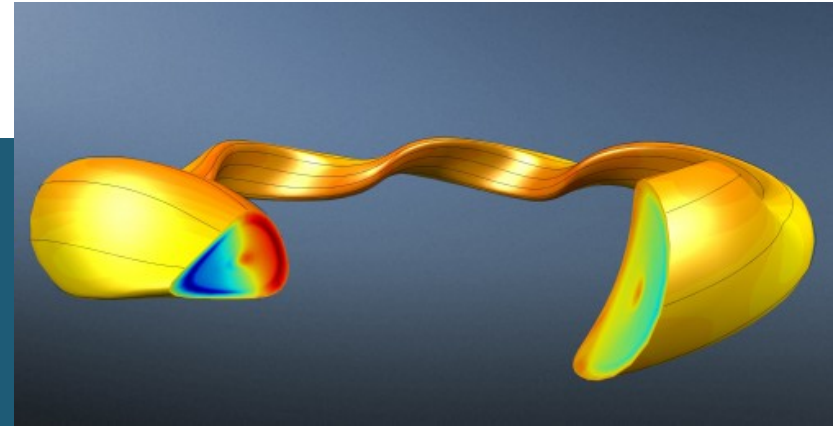


- A brief introduction to the Center and some simple rules for getting work done at NERSC.



Trajectory of an energetic ion in a Field Reverse Configuration (FRC) magnetic field. Magnetic separatrix denoted by green surface. Spheres are colored by azimuthal velocity. Image courtesy of Charlson Kim, U. of Washington; NERSC repos m487, mp21, m1552

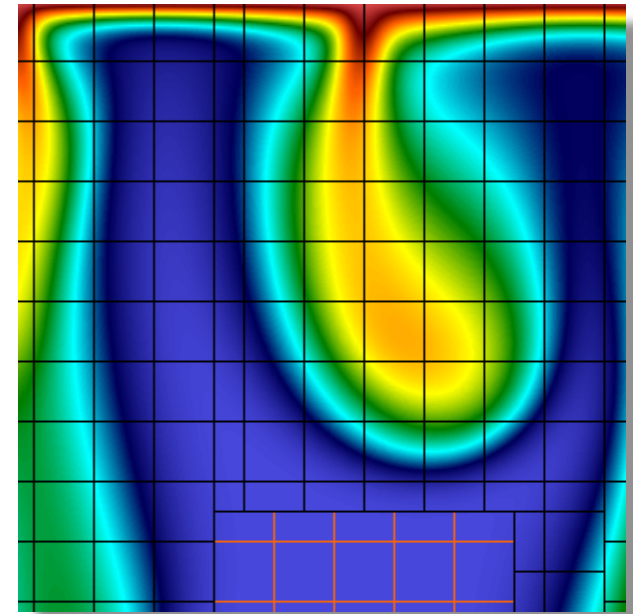
You Are Not Alone!



A calculation of the self-generated plasma current in the W7-X reactor, performed using the SFINCS code on Edison. The colors represent the amount of electric current along the magnetic field, and the black lines show magnetic field lines. Image: Matt Landreman



- **Diverse workload:**
 - 6000 users, 750+ projects
 - 700 codes; 100s of users daily
- **Allocations controlled primarily by DOE**
 - 80% DOE Annual Production awards (ERCAP):
 - From 10K hour to ~10M hour
 - Proposal-based; DOE chooses
 - 10% DOE ASCR Leadership Computing Challenge
 - 10% NERSC reserve
 - NISE, NESAP

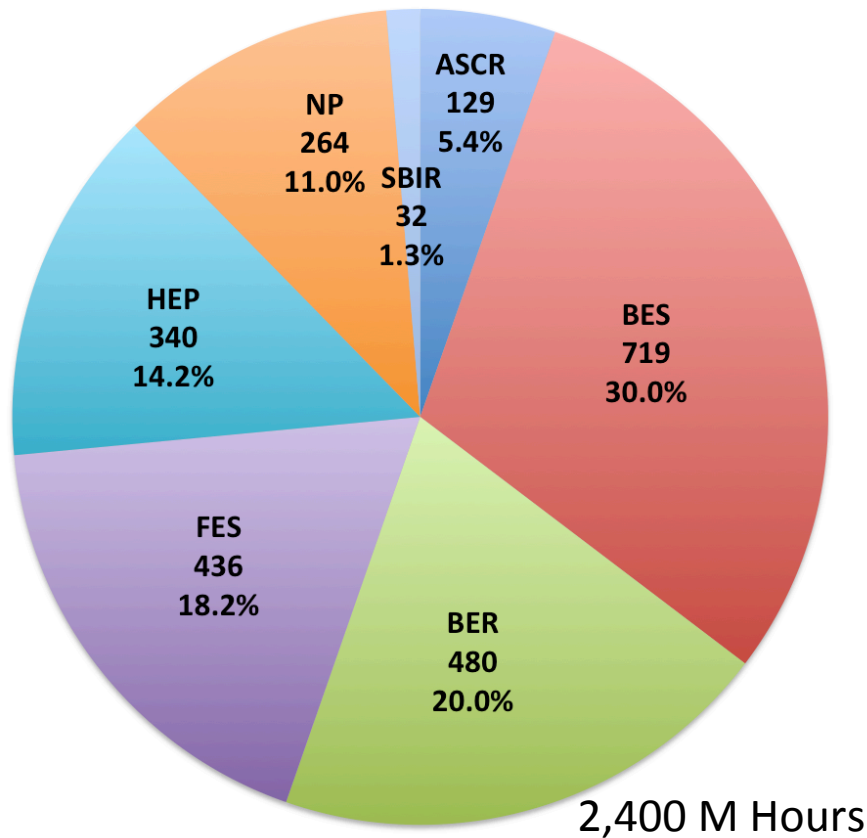


Simulation of density-driven flow for CO₂ storage in saline aquifers. Shown is a snapshot of the CO₂ concentration after onset of convection overlayed on the AMR grid. Image courtesy of George Pau and John Bell (LBNL). Repo mp111

DOE View of Workload



Initial Allocation of Hours by DOE OSc Program Office 2015



ASCR

**Advanced Scientific
Computing Research**

BER

**Biological &
Environmental
Research**

BES

Basic Energy Sciences

FES

Fusion Energy Sciences

HEP

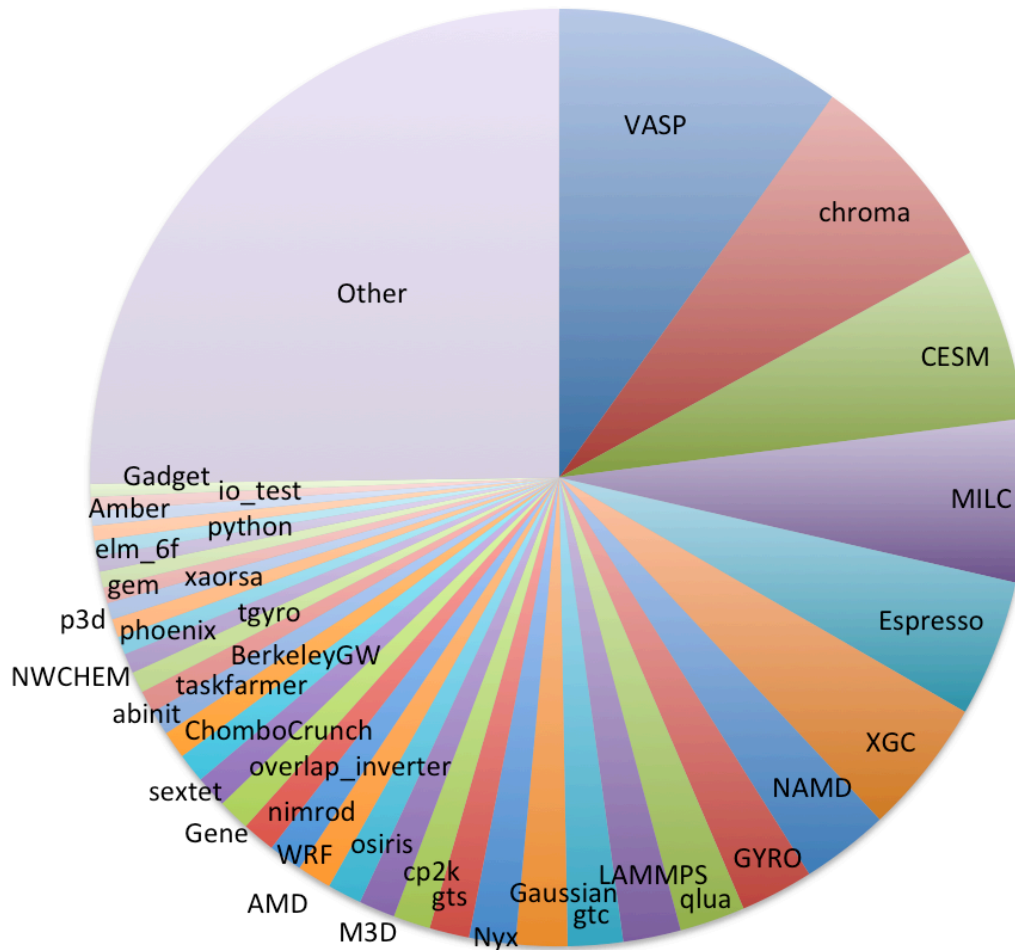
High Energy Physics

NP

Nuclear Physics

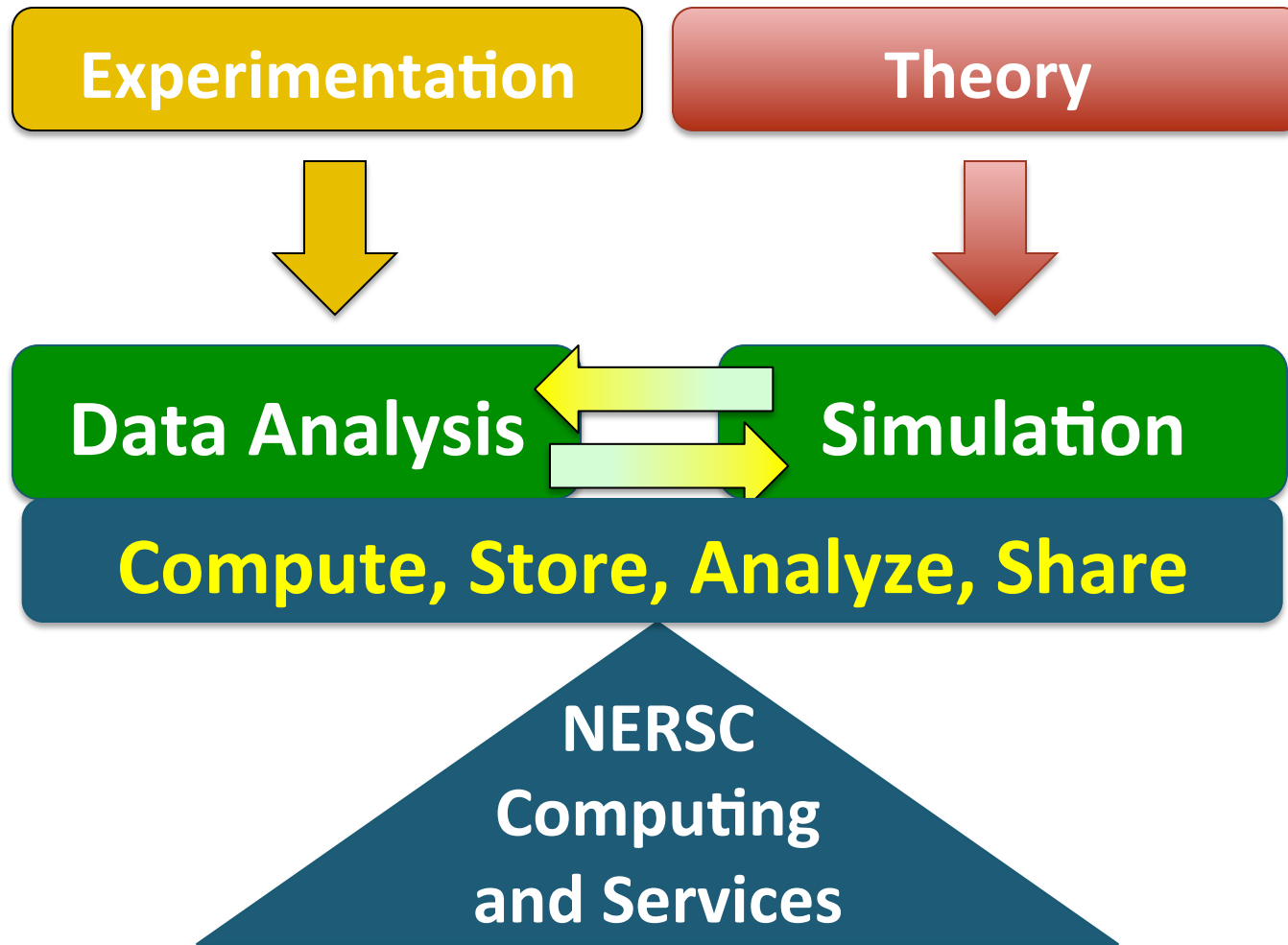
Over 600 codes run at NERSC

NERSC 2015 Code Usage

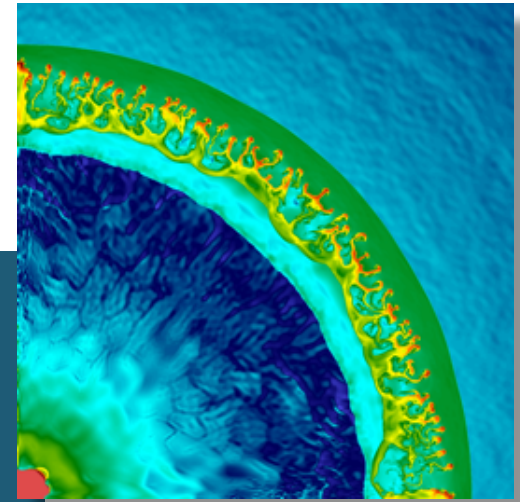


- 10 codes make up 50% of the workload
- 25 codes make up 66% of the workload

What Role Does NERSC Play?



You Will Be Successful!



Collision between two shells of matter ejected in two supernova eruptions, showing a slice through a corner of the event. Colors represent gas density (red is highest, dark blue is lowest). Image courtesy of Ke-Jung Chen, School of Physics and Astronomy, Univ. Minnesota. Repo m1400

2015 Science Output



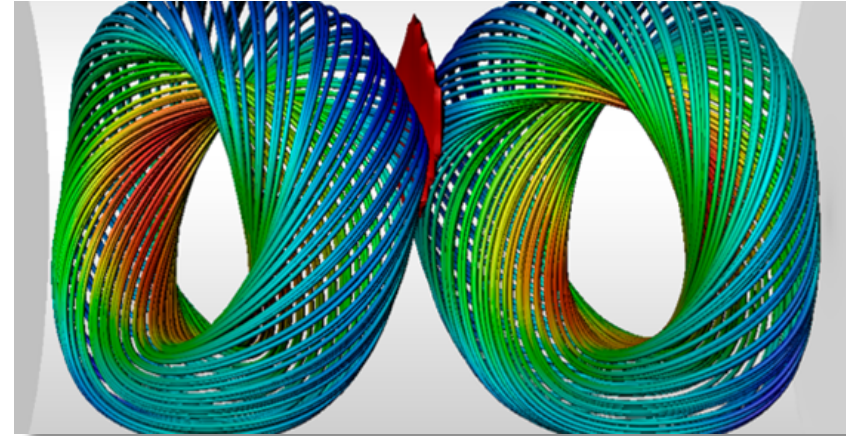
2,078 refereed publications



NERSC Users Report >2000 Publications / Year

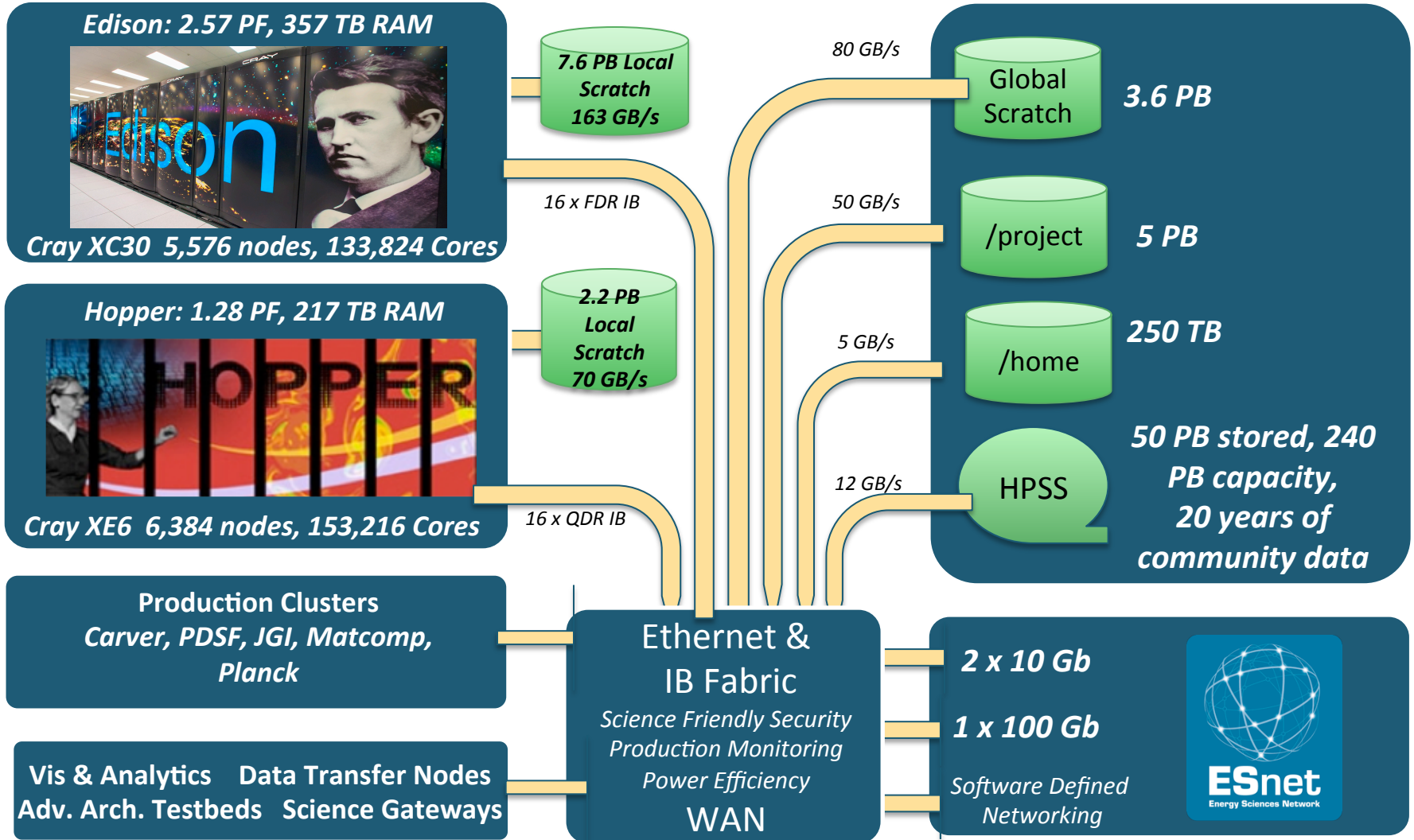


- Make sure you **acknowledge NERSC** in publications; please use “official” acknowledgement
- <https://www.nersc.gov/users/accounts/user-accounts/acknowledge-nersc/>
- *This research used resources of the National Energy Research Scientific Computing Center, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.*
- Science highlights sent to DOE each quarter.
 - Send us links to your publications.



*Magnetic field lines from HiFi simulations of two spheromaks.
NERSC repo m1255
Image courtesy of Vyacheslav Lukin (NRL)*

NERSC Systems Today



Edison

- Largest machine
- Large processor count jobs given priority boost
- 40% discount on very large jobs
- Lower charge factor
- No capability for single-core or serial jobs

Cori

- Throughput machine
- Queues allow single-core jobs
- Longer walltime limits for smaller jobs
- Higher charge factor
- Large processor count jobs discouraged (no boost)

Simple Rules for Success

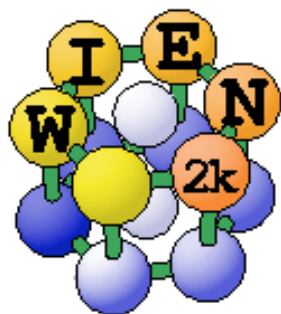


- Use our web site; use “Search...”
- Cray systems are not “typical” clusters, pay attention to differences
- Be kind to your neighbor users
- Back your stuff up
- Pick the right resource for your job and your data
- Use batch system effectively; pay attention to system-specific syntax and policies
- Use your allocation smartly
- Pay attention to security

Chemistry & Materials Applications

NERSC

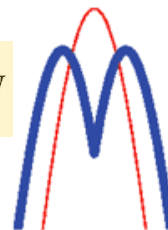
- NERSC compiles and supports many software packages for our users.



BerkeleyGW



QUANTUM ESPRESSO



Molpro

LAMMPS

abinit.

- More than 13.5 million lines of source code Compiled, Optimized, and Tested*



NAMD

Scalable Molecular Dynamics



GÅMESS

GAUSSIAN

Q-CHEM™

WANNIER90

CPMD



NWChem

HIGH-PERFORMANCE COMPUTATIONAL
CHEMISTRY SOFTWARE

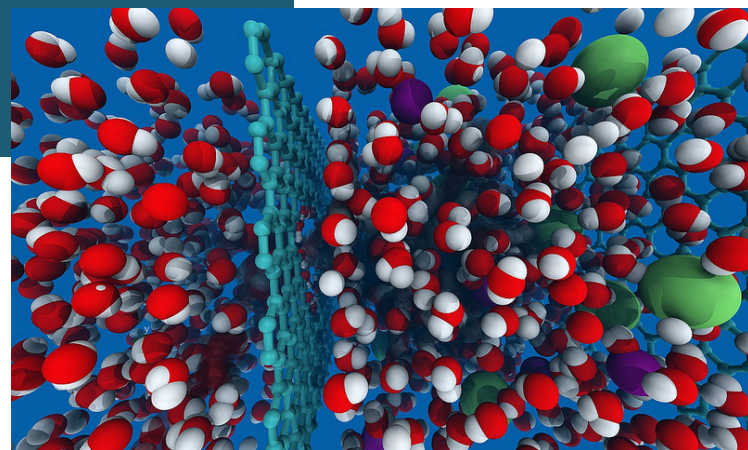


U.S. DEPARTMENT OF
ENERGY

Office of
Science

- **Get involved. Make NUG work for you.**
- **Provide advice, feedback – we listen.**
- **Monthly teleconferences with NERSC, usually the 2nd Thursday of the month, 11:00 AM to noon Pacific Time.**
- **Executive Committee - three representatives from each office and three members-at-large.**
- **Community!**

Rule # 4: Expect Consistency. And Change.



Molecular Dynamics simulation snapshot showing water molecules (red and white), and sodium, chloride ions (green and purple) encountering a sheet of graphene (pale blue, center) perforated by holes of the right size, with water passing through (left side), but sodium and chloride being blocked.

NERSC Timeline



**NRP
complete
12.5 MW**

2015

**Staff
move in**

**NERSC-8
Cori
Phase I**

2016

**Edison
Move
Complete**

**NERSC-8
Cori
Phase II**

**CRT
25MW
upgrade**

2016-18

2020

**NERSC-9
150-300
Petaflops**

**CRT
35+ MW
upgrade**

2021

**NERSC-10
Capable
Exascale
for broad
Science**

2024

2028

**NERSC-11
5-10
Exaflops**



U.S. DEPARTMENT OF
ENERGY

Office of
Science



NERSC

Thank you and welcome to NERSC!

Generic Multiprocessor Architecture

